Trimethoxycinnamaldehyde

Inchi: InChI=1S/C12H14O4/c1-14-10-8-12(16-3)11(15-2)7-9(10)5-4-6-13/h4-8H,1-3H3/b5-4+
InchiKey: DNAVOCNYHNNEQI-SNAWJCMRSA-N
Formula: C12H14O4
SMILES: COc1cc(OC)c(OC)cc1C=CC=O
Mol. weight [g/mol]: 222.24

Physical Properties

Property code	Value	Unit	Source
gf	-200.62	kJ/mol	Joback Method
hf	-453.91	kJ/mol	Joback Method
hfus	25.77	kJ/mol	Joback Method
hvap	60.48	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	1.925		Crippen Method
mcvol	171.060	ml/mol	McGowan Method
pc	2477.65	kPa	Joback Method
rinpol	1845.00		NIST Webbook
rinpol	1845.00		NIST Webbook
tb	635.66	K	Joback Method
tc	844.11	K	Joback Method
tf	392.59	K	Joback Method
vc	0.650	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.76	J/mol×K	635.66	Joback Method
cpg	481.90	J/mol×K	809.37	Joback Method
cpg	471.44	J/mol×K	774.63	Joback Method
cpg	460.29	J/mol×K	739.89	Joback Method
cpg	448.45	J/mol×K	705.14	Joback Method
cpg	435.94	J/mol×K	670.40	Joback Method
cpg	491.65	J/mol×K	844.11	Joback Method
dvisc	0.0001065	Pa×s	635.66	Joback Method

dvisc	0.0001298	Pa×s	595.15	Joback Method
dvisc	0.0001630	Pa×s	554.64	Joback Method
dvisc	0.0002122	Pa×s	514.12	Joback Method
dvisc	0.0002890	Pa×s	473.61	Joback Method
dvisc	0.0004168	Pa×s	433.10	Joback Method
dvisc	0.0006485	Pa×s	392.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R334384&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume